

Fermi Surface and Magnetism in the Kondo lattice: a Continuum Field Theory Approach

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Abstract

We consider the Fermi surface inside the antiferromagnetic ordered region of a Kondo lattice system in an arbitrary dimension higher than one. We establish the existence of AF_S, an antiferromagnetic phase whose Fermi surface is “small,” in the sense that the local moments do not participate in the Fermi-surface formation. This is in contrast to the “large” Fermi surface that is typically assumed for heavy fermion metals. We extend our earlier work to the case that the Fermi surface of the conduction electrons intersects the antiferromagnetic Brillouin zone boundary. Our results provide a new perspective on local quantum criticality. In addition, our results imply that, for the AF_S phase, it is important to keep track of the dynamical screening processes; we suggest that this effect is not captured in a recent variational Monte-Carlo study of the Kondo lattice.

Key words: Kondo lattice; Fermi surface; Antiferromagnetism; Quantum phase transitions

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Quantum criticality and the associated magnetic quantum phases of heavy fermion metals are of extensive current interest, and the nature of the Fermi surface has emerged as an important characterization of both[1,2]. This is because the presence or absence of Kondo screening, which influences quantum criticality, also leads to distinct Fermi surfaces in the proximate zero-temperature phases[3]. In order to elucidate these issues, we study the Kondo lattice model deep in its antiferromagnetic (AF) phase, in terms of a quantum nonlinear sigma model (QNLσM) representation of the local-moment component[4]. We end up with an effective coupling between the spin waves and conduction electrons, which we show is exactly marginal in the renormalization group (RG) sense.

The Kondo lattice model is defined by: $\mathcal{H} = \mathcal{H}_c + \mathcal{H}_f + \mathcal{H}_K$, where, in standard notation, $\mathcal{H}_c = \sum_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$ for a band of conduction c -electrons, $\mathcal{H}_f = (1/2) \sum_{ij} I_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$ for a lattice of spin-1/2 f -moments, and $\mathcal{H}_K = \sum_i J_K \mathbf{S}_i \cdot \mathbf{s}_{c,i}$ describes the Kondo interaction. We will focus on the AF Kondo lattice model, with the dominant nearest-neighbor RKKY interaction I being antiferromagnetic ($I > 0$), as is the Kondo interaction ($J_K > 0$). We consider the situation deep inside the AF part of the $T = 0$ phase

diagram, where $J_K \ll I$ and both are much smaller than the bandwidth of the conduction electrons.

Since we are dealing with the ordered phase of a local moment antiferromagnet rather than a single impurity spin, we map \mathcal{H}_f to a QNLσM by standard means[5,6]: $2\mathbf{S}_i \rightarrow \eta_{\mathbf{x}} \mathbf{n}(\mathbf{x}, \tau) \sqrt{1 - [2a^d \mathbf{L}(\mathbf{x}, \tau)]^2} + 2a^d \mathbf{L}(\mathbf{x}, \tau)$, where \mathbf{x} labels the position, $\eta_{\mathbf{x}} = \pm 1$ on even and odd sites, and a is the lattice constant. The low-lying excitations are concentrated in the momentum space near $\mathbf{q} = \mathbf{Q}$ (the AF wavevector) and $\mathbf{q} = \mathbf{0}$, corresponding to \mathbf{n} and \mathbf{L} respectively.

The case with the Fermi surface of the conduction electrons not intersecting the antiferromagnetic Brillouin zone (AFBZ) boundary was treated in Ref. [4]. Here, the linear coupling $\mathbf{n} \cdot \mathbf{s}_c$ cannot connect two points on the Fermi surface and thus, for low energy physics, it does not come into play. The Kondo coupling reduces to, $\mathbf{S} \cdot \mathbf{s}_c \rightarrow a^d \mathbf{L} \cdot \mathbf{s}_c$, corresponding to forward scattering for the conduction electrons. Integrating out the \mathbf{L} field leads to the effective action: $\mathcal{S} = \mathcal{S}_{\text{QNL}\sigma\text{M}} + \mathcal{S}_{\text{Berry}} + \mathcal{S}_K + \mathcal{S}_c$, where $\mathcal{S}_{\text{QNL}\sigma\text{M}}$ is the quantum non-linear sigma model and \mathcal{S}_c the action for a free fermion band with a dispersion of $\xi_K \equiv v_F(K - K_F)$. The Kondo coupling has the form $\mathcal{S}_K = \lambda \int d^d x d\tau [\mathbf{s}_c(\mathbf{x}, \tau) \cdot \boldsymbol{\varphi}(\mathbf{x}, \tau)]$, where the vector boson field $\boldsymbol{\varphi}$ represents $\mathbf{n} \times \frac{\partial \mathbf{n}}{\partial \tau}$, with \mathbf{n} being the QNLσM field. The constraint $\mathbf{n}^2 = 1$ is implemented by $\mathbf{n} = (\boldsymbol{\pi}, \sigma)$, where $\boldsymbol{\pi}$ labels the Goldstone magnons and $\sigma \equiv \sqrt{1 - \boldsymbol{\pi}^2}$ is the mas-

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sive field. The Berry phase term, $\mathcal{S}_{\text{Berry}}$, is not important inside the Néel phase.

In order to keep track of the Fermi surface in the RG procedure, we use a combination of the fermionic RG [7] and standard bosonic RG methods. We find a marginal coupling at the tree level: the scaling dimension $[\lambda] = 0$. It turns out that certain kinematic restrictions prevent higher-loop corrections from entering the beta function. This results from the forward-scattering nature of the effective Kondo coupling. At the one-loop level this can be seen by an explicit calculation, where momentum conservation inside the restrictive cutoffs limits the region of integration to an area of size $(d\Lambda)^{3/2}$. (Here $d\Lambda = \Lambda - \Lambda/s$, in the $s \rightarrow 1^+$ limit.) Going beyond one loop, it turns out that the Kondo vertex contains a small parameter, $1/N_\Lambda \equiv \Lambda/K_F$, relative to the kinetic term: $\mathcal{S}_K/\mathcal{S}_c \propto 1/\sqrt{N_\Lambda}$ in the spin-flip case, and $\mathcal{S}_K/\mathcal{S}_c \propto 1/N_\Lambda$ in the longitudinal case. In the asymptotic low-energy limit ($N_\Lambda = \infty$), the higher loop corrections to the beta function vanish. Therefore, the one-loop result is the whole story and the Kondo coupling is exactly marginal. There is no flow to the strong-coupling fixed point. This implies the absence of static Kondo screening, and the Fermi surface remains small. It also means that there is no singular correction to the QNL σ M itself. Both conclusions can also be seen in a suitable large- N limit of the effective action[4].

We now turn to the case when the Fermi surface of the conduction electrons intersects the AFBZ boundary. Here, the linear coupling $\mathbf{n} \cdot \mathbf{s}_c$ cannot be neglected. The AF order of the local moments implies that a staggered field is applied to the conduction electrons, resulting in a reconstruction of their Fermi surface: the hot spots of the Fermi surface become gapped out, as shown in Fig. 1. At the mean field level, the conduction electron component now becomes:

$$\mathcal{H}_c^{\text{MF}} = \sum_{k\alpha\beta}^{AFBZ} \begin{pmatrix} c_{k,\alpha}^\dagger & c_{k+Q,\alpha}^\dagger \end{pmatrix} \begin{pmatrix} \tau_{\alpha\beta}^0 \epsilon_k & \tau_{\alpha\beta}^z \Delta \\ \tau_{\alpha\beta}^z \Delta & \tau_{\alpha\beta}^0 \epsilon_{k+Q} \end{pmatrix} \begin{pmatrix} c_{k,\beta} \\ c_{k+Q,\beta} \end{pmatrix}$$

where the sum on k only runs over the AFBZ, $\mathbf{Q} = (\pi/a, \pi/a)$ is the AF ordering wavevector, $\tau^{0,z}$ are the 2×2 unit/Pauli matrices, and the gap is given by the product of the Kondo coupling and expectation value of the massive field of the QNL σ M: $\Delta = \lambda \langle \sigma \rangle$. This is simply diagonalized by a unitary transformation:

$$\begin{pmatrix} a_{k\alpha} \\ b_{k\alpha} \end{pmatrix} = \begin{pmatrix} u_k \sigma_{\alpha\beta}^0 & v_k \sigma_{\alpha\beta}^z \\ v_k \sigma_{\alpha\beta}^z & -u_k \sigma_{\alpha\beta}^0 \end{pmatrix} \begin{pmatrix} c_{k\beta} \\ c_{k+Q,\beta} \end{pmatrix}. \quad (1)$$

Using these new quasiparticles, the effective spin-flip Kondo couplings become

$$-\frac{J_K}{2} \sum_k \sum_q^{AFBZ} \left[\Gamma^{\sigma\bar{\sigma}}(k, q) \left(a_{k\sigma}^\dagger a_{k+q,\bar{\sigma}} - b_{k\sigma}^\dagger b_{k+q,\bar{\sigma}} \right) n_q^{\bar{\sigma}} \right] \quad (2)$$

where $\Gamma^{\sigma\bar{\sigma}}(k, q) = u_k v_{k+q} - v_k u_{k+q}$ is the coherence factor. The other terms, such as inter-band interactions (e.g. $a^\dagger b$) are gapped out at low energies. Near the ordering wavevector the vertex is linear in momentum: $\Gamma^{\uparrow\downarrow}(k, q) \propto q$, where

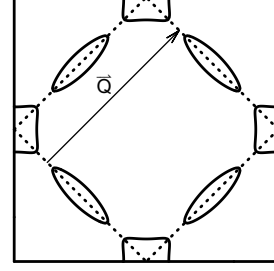


Fig. 1. When the Fermi surface of the conduction electrons intersects the AFBZ boundary (the dashed lines), the Kondo coupling connects the re-diagonalized fermions (whose Fermi surfaces are given by the solid lines) to the QNL σ M fields.

q is the deviation from the AF ordering wavevector \mathbf{Q} . (See e.g., Ref. [8].) The form of this linear-momentum suppression factor survives beyond the mean-field treatment of the conduction electron band, as dictated by Adler's Theorem. Within the RG analysis, the linear-momentum factor serves the same function as the time derivative in φ to preserve the marginality of the transverse Kondo coupling.

The marginal nature of the Kondo coupling means that the effective Kondo coupling is finite at finite energies in the AFs phase. One corollary is that the ground state wavefunction will incorporate such dynamical screening effects. Recently, Watanabe and Ogata [10] have carried out a variational Monte-Carlo study of the Kondo lattice. Their choice of the variational wavefunction for the AFs does not contain any dynamical screening, which we believe is responsible for their finding that the AFs phase is energetically unfavorable.

In conclusion, we have shown that the Kondo coupling deep inside the ordered region of the antiferromagnetic Kondo lattice is exactly marginal, thereby establishing the existence of an antiferromagnet with a small Fermi surface. The stability of this AFs phase provides a new anchoring point to view the destruction of Kondo effect at the magnetic quantum critical point, as given in the local quantum criticality [9]. It also serves as a benchmark for any approximate or numerical studies of the Kondo lattice model.

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References

- [1] S. Paschen *et al.*, Nature **432** (2004) 881.
- [2] H. Shishido *et al.*, J. Phys. Soc. Jpn. **74** (2005) 1103.
- [3] Q. Si, Physica B **378** (2006) 23.
- [4] S. J. Yamamoto and Q. Si, Phys. Rev. Lett. **99** (2007) 016401.
- [5] F. D. M. Haldane, Phys. Rev. Lett. **50** (1983) 1153.
- [6] S. Chakravarty *et al.*, Phys. Rev. B **39** (1989) 2344.
- [7] R. Shankar, Rev. Mod. Phys. **66** (1994) 129.
- [8] I. Vekhter and A. V. Chubukov, Phys. Rev. Lett. **93** (2004) 016405.
- [9] Q. Si *et al.*, Nature (London) **413** (2001) 804.
- [10] H. Watanabe and M. Ogata, arXiv:0704.1722.